On Improving the Performance of an Iterative Linear Solver

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Can we solve large, sparse systems of linear equations more efficiently?

- linear system: $\mathbf{Ax} = \mathbf{b}$

  ($\mathbf{A}$ is large, sparse, and nonsymmetric)

- costs: (1) floating-point operations (FLOPs)

  (2) movement of data through memory

- iterative linear solver: GMRES(m)

  (restarted Generalized Minimum Residual method)

Motivation

- linear systems are often time-consuming to solve
- GMRES(m) convergence can be slow
- moving data is expensive
  - iterative linear solvers:

    access $\mathbf{A}$ once per iteration loop for $\mathbf{A} * \mathbf{x}$

Memory costs impact performance

memory hierarchy component	typical CPU latency value
L1 cache	1 - 3 cycles
L2 cache	6 - 20 cycles
main memory	60 - 140 cycles
disk	10,000 cycles!!!

- getting worse: improvement in

  microprocessor performance vs. memory performance:
  $\sim$ 60% per year $<$ 10% per year

- memory costs >> FLOP costs for large problems

Approach for improving GMRES(m)

(1): FLOPs

- improve convergence behavior $\Rightarrow$ reduce the number of iterations

(2): data movement

- reformulate algorithm to reduce data movement

$$\begin{bmatrix} \\ \mathbf{A} \\ \\ \end{bmatrix} \begin{bmatrix} \\ \mathbf{x} \\ \\ \end{bmatrix} = \begin{bmatrix} \\ \mathbf{b} \\ \\ \end{bmatrix} \quad \Rightarrow \quad \begin{bmatrix} \\ \mathbf{A} \\ \\ \end{bmatrix} \begin{bmatrix} \\ \mathbf{X} \\ \\ \end{bmatrix} = \begin{bmatrix} \\ \mathbf{B} \\ \\ \end{bmatrix}$$

- "smart" implementation

Accelerating convergence

- augmented methods

  (Morgan '95, '00, Chapman and Saad '97)

  – add additional vectors to Krylov subspace

- nested Krylov (truncated)

  (Van der Vorst and Vuik '94, de Sturler '96 and '99)

  – approximately solve residual equation ($Ae = r_i$)

- LGMRES

  (Baker, Jessup, Manteuffel)

  – combination of the approaches above

What should we choose for B for GMRES(m)? ($\mathbf{Ax = b \Rightarrow AX = B}$)

- goal:
  balance memory-usage and favorable numerical properties

- observation:
  restarted GMRES(m) throws away useful information with every restart, which slows convergence

- our approach:
  compensate for this loss $\rightarrow$ put the lost information in B!

$\mathbf{Ax = b \Rightarrow AX = B}$

GMRES(m):

- restart cycle $\mathbf{i}$: $\mathbf{x_i = x_{i-1} + c}, \quad \mathbf{c \in \mathcal{K}_m(A, r_{i-1})}$
- ideally: $\mathbf{c = x_{exact} - x_{i-1} \longrightarrow x_i = x_{exact}}$
- error approximation: $\mathbf{z_i \equiv x_i - x_{i-1}}$

idea:

- put the error approximation vector in $\mathbf{B}$: $\mathbf{B = [\, b\,,\, z_i\,]}$

A new algorithm: B-LGMRES

B-LGMRES(m, 1):

- restart cycle $\mathbf{i+1}$: $\mathbf{Ax = b \Rightarrow AX = B}$

  $\mathbf{X = [\, x_i\,,\ 0\,]}$ (initial guess)

  $\mathbf{B = [\, b\,,\ z_i\,]}$ (right-hand side)

  i.e., augment $\mathbf{b}$ with an error approximation

  $(\mathbf{z_i \equiv x_i - x_{i-1}})$

- $\underline{\mathbf{x_{i+1} \in x_i + \mathcal{K}_m(A, r_i)}} + \mathcal{K}_\mathbf{m}(\mathbf{A}, \mathbf{z_i})$

  $\|$

  GMRES(m)

B-LGMRES: an efficient implementation

Matrix-multivector multiply (Kaushik '99):

multiply $\mathbf{A}$*4 vectors in $\approx$ 1.5 the time for $\mathbf{A}$*1 vector

- process the vectors in groups or "multivectors"
- interleave the vector components in memory

  e.g., $\mathbf{v_1(j)}$, $\mathbf{v_2(j)}$, $\mathbf{v_3(j)}$, $\mathbf{v_4(j)}$ are adjacent (row-wise)
- unroll the inner matrix multiplication loop
  (across multivector elements)

Evaluating the new method:

B-LGMRES(15, 1) vs. GMRES(30):

- equal approximation space size (30)
- variety of problems from several test collections
- problem size: $n = 7,740$ to $1,709,982$
  ($nnz = 79,566$ to $1,717,792$)
- either ILU preconditioner or no preconditioner
- Argonne's PETSc with modifications

Some results...

$\Rightarrow$ the new method (B-LGMRES) is generally faster

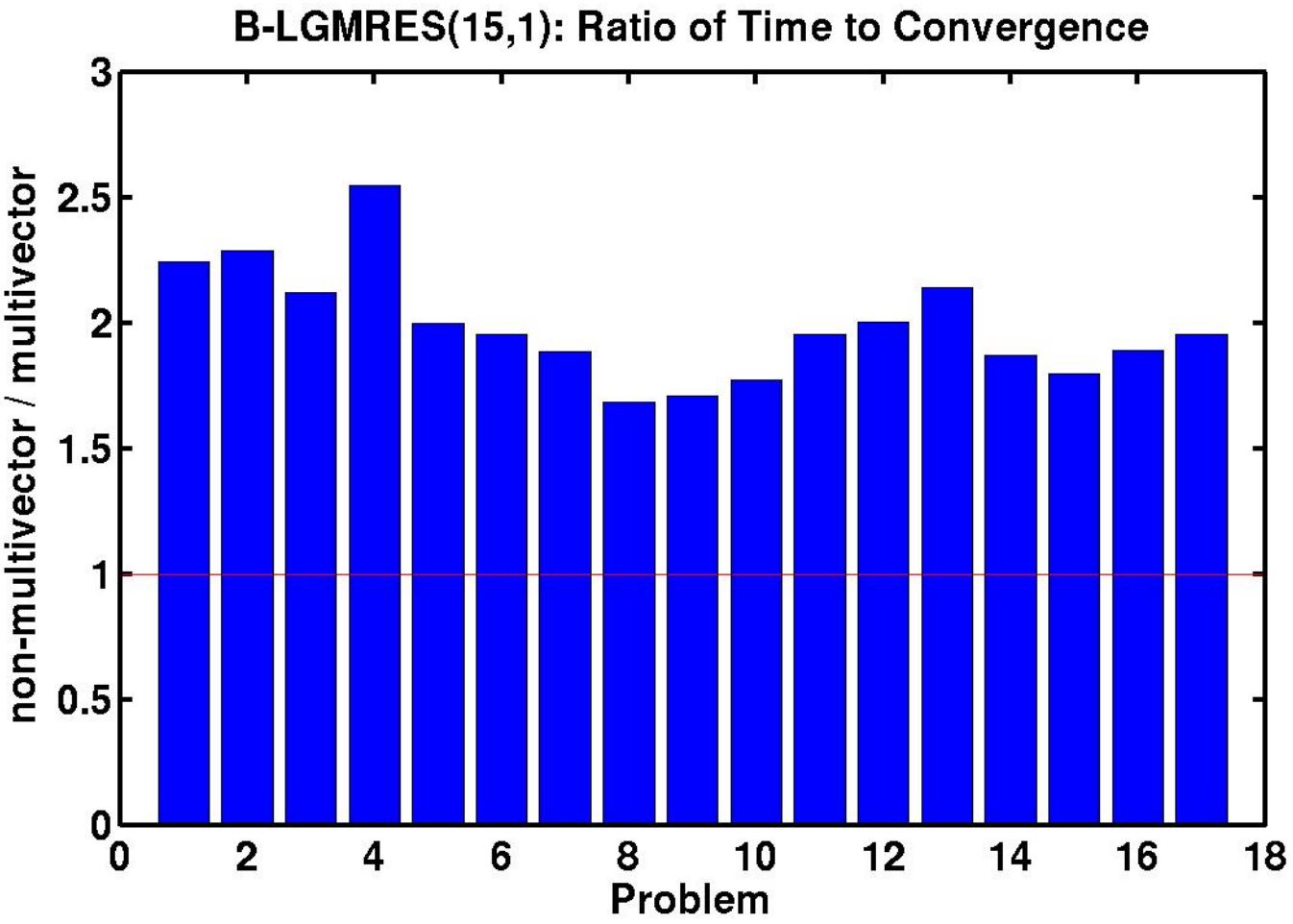
Problem 12: 2-D fluid flow

size: n=13,535, nnz=390,607

method	execution time	accesses of $\mathbf{A}$	matrix-vector multiplies
GMRES(30)	$165.9 \pm .6$ s	1960	1960
B-LGMRES(15,1)	$78.5 \pm .2$ s	1004	2008

$\Rightarrow$ execution time correlates to number of accesses of $\mathbf{A}$
(related to memory usage, not floating-point operations)

Importance of an efficient implementation



Conclusions

(1): FLOPs

- accelerate GMRES(m) convergence by preventing repetitiveness

(2): data movement

- algorithmic changes: changing b to B
- implementation: basic programming tricks

$\Rightarrow$ modifying a linear solver to reduce data movement is a viable approach to gaining efficiency!